Relating turbulent premixed flame experiments to detailed simulations. Who cares?

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What's the question?

Say I could hand you a fully resolved numerical simulation of your laboratory experiment. What questions would you ask?

Computation has entered a new era. Can we think of a new way to couple simulation and experiment to really take these studies to the "next level"? (and, by the way, what *is* the next level?)

Are there sources of error in my calculations that are relevant to a larger community, such that reducing them helps everyone?

Simulation elements

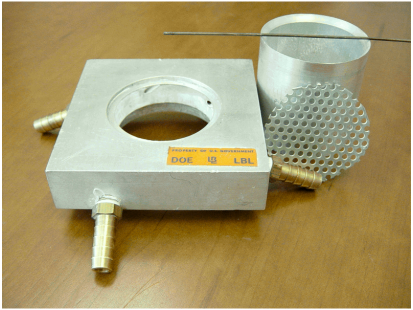
Observation:

- Open laboratory turbulent flames are low Mach number
- Regions requiring high-resolution are localized in space

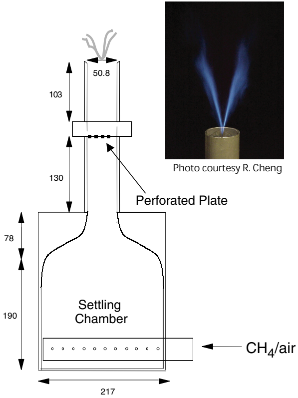
Our approach:

- Low Mach number formulation
  - Eliminate acoustic time-step restriction while retaining compressibility effects due to heat release
  - Conserve species and enthalpy
- Adaptive mesh refinement
  - Localize mesh where needed
  - Complexity from synchronization of elliptic solves
- Parallel architectures
  - Distributed memory implementation
  - Dynamic load balancing of heterogeneous work load

Laboratory-scale V-flame



Burner assembly



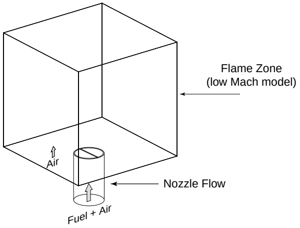
Experiment schematic

- V-flame ($\dot{m}_{air} \equiv 0$): rod $\sim$ 1 mm
- Turbulence plate: 3 mm holes on 4.8 mm center

V-flame Setup

Simulation Strategy

Treat nozzle exit as inflow boundary condition for low Mach number combustion simulation



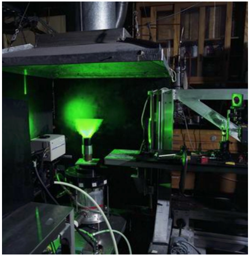
Reacting flow simulations

- 12cm x 12cm x 12cm domain
- DRM-19: 20 species, 84 reactions
- Mixture model for differential diffusion

Nozzle inflow simulations

- Mean flow
  - 3 m/s mean inflow
  - Boundary layer profile at edge
  - Noflow condition to model rod
  - Weak co-flow air
- Turbulent fluctuations
  - $\ell_t = 3.5$ mm, $u' = 0.18$ m/s
  - Estimated $\eta = 220\mu$m

Characterizing the flame surface



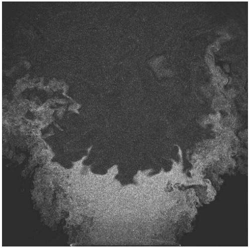
- PIV laser: double pulses
- 2000×2000 pixel camera
- 11×11 cm field of view
- 0.3 μm Al_2O_3 particles
- Time separation 35 μsec
- Analysis: 64×64 subregion (3.6 mm)

Flame surface: jump in particle density

Velocity: frame correlation

Limitations

1. Resolution: radical zone < 200 μm
2. Transient and 3D effects “difficult”

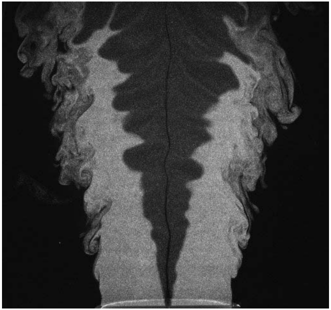


Sample PIV image (LSB)

Results: Computation vs. Experiment

Bell et al., PNAS, **102**(29), 10006-10011 (2005)

CH_4 from simulation

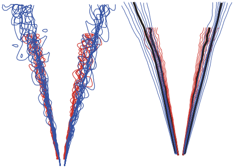


Single image from experimental PIV

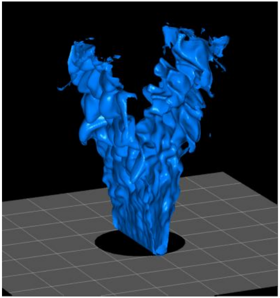
Flame Surface Evolution

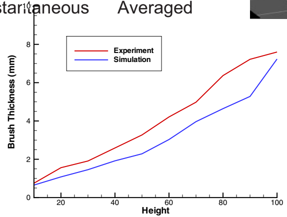
Flame Surface

Red = Experimental
Blue = Simulated



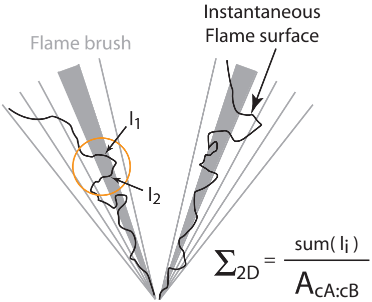
Instantaneous Averaged

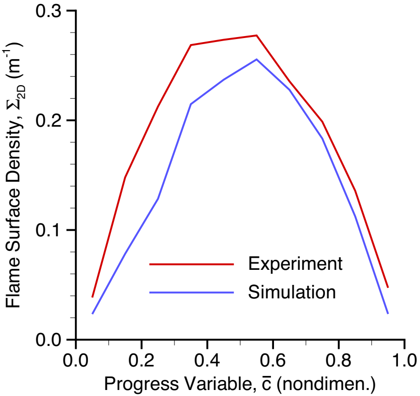




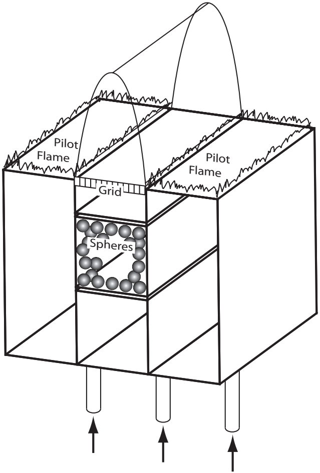
2D Flame Surface Density

Flame surface density in the diagnostic plane





A slot flame

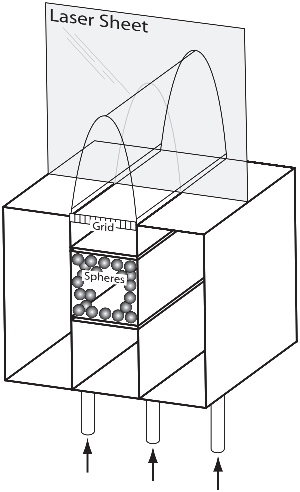


- Slot dimension: 2.5 $\times$ 5 cm (x3)
- Center slot: Turbulent fuel
  - CH_4/air ($\phi = 1$)
  - Mean inflow: 3 m/s
  - Integral scale: 5.2 mm
  - Intensity: 10%
  - Kolmogorov scale: 200 μm
- Side slots: Laminar pilots
  - Burner stabilized flames
  - Isolate flame from lab
  - Flow rate to minimize shear

Experimental Diagnostics, progress variable c

1. Mie-scattering based on oil droplets
   - Flame surface identified where droplets evaporate ($\sim$ 650K)
   - Binarized, averaged to obtain mean, $\bar{c}$
   - Polynomial fit to c interface to obtain "2D curvature"
   - c interface binned in plane to obtain flame surface density Σ_{2D}
   - Flame brush thickness: FWHM of c'_{rms}

2. PLIF imaging of CH fluoresence:
   - Nd:YAG pumped dye laser, 390 nm
   - Alternative flame length measure
     - Binarize PLIF image
     - Area of "on" pixels / δ_{CH} (δ_{CH} mean CH profile thickness)



Mean flame shape is approximately parabolic

Filatyev, *et al.*, Comb. Flame **141** 1–21 (2005)

Simulation parameters

Nozzle (fuel):

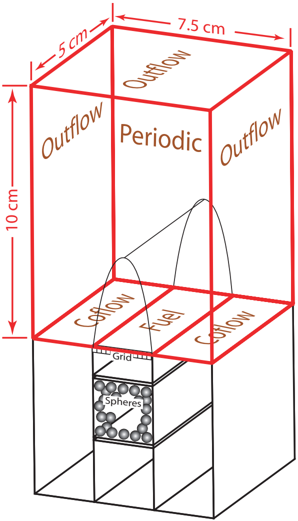
- $\phi = 1$, CH_4-air, $\bar{u} = 3$ m/s*
- Treat as t-dep boundary values
- Evolve fluctuations separately, match experimental (ℓ_t, u')*

Coflow (pilot):

- Hot products at 7 m/s*

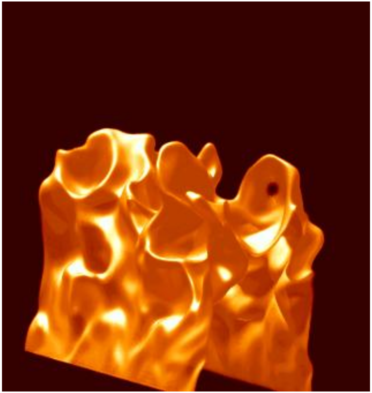
Model:

- DRM-19 (20 species + 84 rxns)
- 3-level dynamic AMR hierarchy
  - 625 μm downstream, coflow
  - 312.5 μm on inlet turbulence
  - 156.25 μm at flame surface

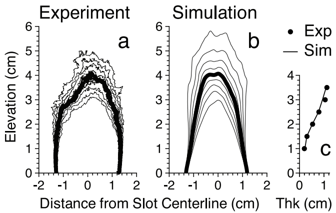


** More detail in these characterizations is desireable*

Flame surface



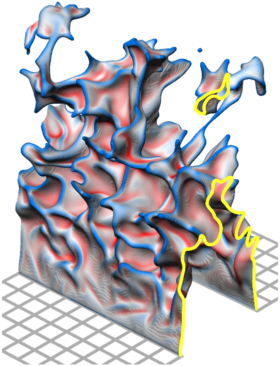
Simulated flame surface



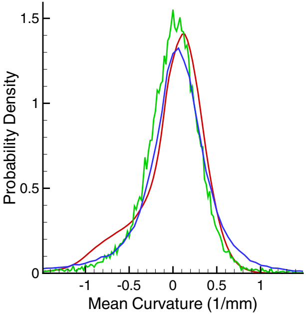
Mean reaction progress, brush thickness

- Turbulent flame speed: expt / sim $\sim$ 1.04
- Brush width agrees for z<3.5 cm

Slot Flame Curvature Statistics



Flame snapshot colored by mean surface curvature



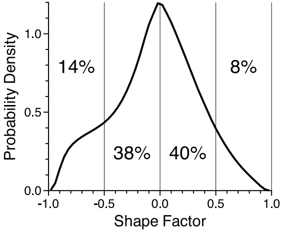
Mean curvature (B=2D, R=3D, G=Expt)

Note: If surface randomly oriented, predict 2D curvatures much higher than 3D. The plot suggests preferred orientation

Shape factor from simulation

Shape factor is an indicator of local flame shape, and has been used to argue whether a flame is 'mostly 2D-like'.

R_1 and R_2 are the principal radii of curvature of a progress isopleth in the flame zone. Integrating over all statistically stationary data



PDF of shape factor

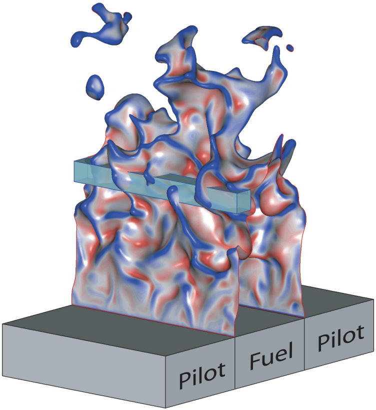
$$S = \begin{cases} R_1/R_2 & \text{if } |R_1| < |R_2| \\ R_2/R_1 & \text{otherwise} \end{cases}$$

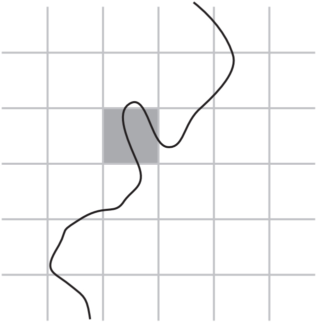
Pope, et al., Phys. Fluids A 1:2010-2018 (2003)

- $S = -1$ local saddles
- $S = +1$ locally spherical
- $S = 0$ local cylindrical

Although S peaked at 0, a significant fraction of the flame has has $|S| > 0.25$

2D and 3D flame surface density

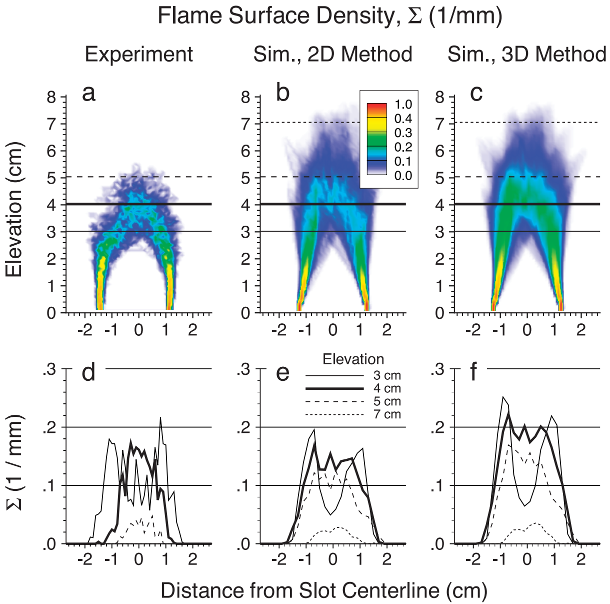




$$\Sigma = \frac{\text{flame area}}{\text{bin volume}}$$

$$\Sigma_{2D} = \frac{\text{flame length}}{\text{bin area}}$$

Flame Surface Density



Descrepancies with comparisons

The computed flame surface statistics are numerically resolved

- Further grid refinements, no changes in statistics
- The flame brush growth, mean flame height, 2D curvature and flame surface statistics show reasonable agreement with experimental data, and the turbulent burning speed is accurately predicted.

However the mean flame shape shows clear descrepancies

- The experimental flame is more squared off, consistent with a poorly characterized mean inflow
- We find flame shape sensitive to U_{coflow} as well

More detail is necessary to characterize the boundary data (mean fuel inflow and fluctuation spectra)

General sources of discrepancy

In general, in trying to match simulation to experiment, there are several classes of “error” or discrepancy which must be addressed:

1. Model assumptions, discretization errors due to under-resolution (though under control here)
2. Input databases (and parameterizations) for chemical kinetics, thermodynamics, multi-species transport
3. Configuration errors, such as inlet turbulence characterization, the “laboratory response” of an unconfined flame, stabilization mechanisms
4. Data extraction from experimental observation, line-of-sight, plane-projected 3D fields, signal modification (PLIF quenching)

The questions for discussion

- How can we more closely couple laboratory experiments and these detailed numerical solutions in a way that makes a real difference?
- Can we "close the loop" between kinetic models of chemistry and transport, and their implementation in more industrially relevant scenarios (like turbulent premixed combustion?
- Is the answer that these simulations are really only good for calibrating LES and RANS models??

The AMR low Mach number tool was developed under DOE MICS funding. The simulations were performed at LBNL on Jaquard and Bassi, and were supported under the SciDAC Program.